

Mass and Density, Criticality Relationships, Generalized

by
Dermott E. Cullen
University of California
Lawrence Livermore National Laboratory
P.O.Box 808/L-159
Livermore, CA 94550

Tele: 925-423-7359 E.Mail: <u>cullen1@llnl.gov</u> Website: <u>http://www.llnl.gov.cullen1</u>

June 30, 2004

U.S. Department of Energy



Approved for public release; further dissemination unlimited.

DISCLAIMER

This document was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the University of California nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or the University of California, and shall not be used for advertising or product endorsement purposes.

Work performed under the auspices of the U. S. Department of Energy by the University of California Lawrence Livermore National Laboratory under Contract W-7405-Eng-48.

This report has been reproduced directly from the best available copy.

Available to DOE and DOE contractors from the Office of Scientific and Technical Information P.O. Box 62, Oak Ridge, TN 37831 Prices available from (423) 576-8401 http://apollo.osti.gov/bridge/

Available to the public from the National Technical Information Service U.S. Department of Commerce 5285 Port Royal Rd.,
Springfield, VA 22161
http://www.ntis.gov/

OR

Lawrence Livermore National Laboratory
Technical Information Department's Digital Library
http://www.llnl.gov/tid/Library.html

Mass and Density, Criticality Relationships, Generalized

by
Dermott E. Cullen
University of California
Lawrence Livermore National Laboratory
P.O.Box 808/L-159
Livermore, CA 94550

Tele: 925-423-7359 E.Mail: <u>cullen1@llnl.gov</u> Website: http://www.llnl.gov.cullen1

Overview

As it relates to neutron transport calculations, in an earlier report [1] I defined scaling laws relating reactivity or criticality to the mass, density and dimensions of geometrically simple systems. Here I generalize these scaling laws to any geometry. These are well known relationships that allow the variation of critical mass versus density and/or dimensions to be written in a simple analytical form. With these relationships anyone can quickly estimate the critical mass corresponding to any given density, using nothing more complicated than a hand calculator. In addition I point out that these scaling laws can be used to easily predict the sensitivity of a system's K-eff to variations in density and/or dimensions.

These relationships have appeared extensively in the literature for over 50 years, but seem to be periodically forgotten. As such, this report is not intended to present any new information, but rather it is intended merely to refresh our memories. The main idea is that you do not have to perform neutron transport calculations every time a parameter of a system is changed; instead you can use simple scaling laws to determine what will change. Here is a quick summary of results,

First let's discuss systems in which we constrain the product of density ρ and linear dimension R, to remain constant, i.e., any change in ρ is exactly compensated by a change in R, such that the product $\rho * R$ remains constant.

1) **K-eff:** For any given system, a variation in density ρ and linear dimension R, such that the product $\rho * R$ remains constant, will have exactly the same K-eff. For example, if I start from one given system and I double the density of the system and half all of its dimensions to create a new system, the new system will have exactly the same K-eff as the original system.

K-eff = $C^* \rho * R$, C is the constant of proportionality, to be determined

2) **Time Constant** (α): For any given system, a variation in density ρ and linear dimension R, such that the product ρ^*R remains constant, the time constant will vary directly with the density ρ . For example, if I start from a given system and I double the density of the system, the time constant (α) will also double, because in the new system everything will happen twice as fast. Note, since we are only considering systems where ρ^*R is constant, if we double the density ρ we must be halving the linear dimension R, so we obtain two relationships,

 $\alpha = D^* \rho = E/R$, D and E are constants of proportionality, to be determined

3) **Mass:** For any given system, a variation in density ρ and linear dimension R, such that the product $\rho * R$ remains constant, the critical mass of the system will vary inversely with the square of the density ρ . For example, if I start from a given system and I double the density the critical mass will be one fourth. Note, since we are only considering systems where $\rho * R$ is constant, if we double the density ρ we must be halving the linear dimension R, so we obtain two relationships,

Mass = A/ ρ^2 = B*R², A and B are constants of proportionality, to be determined

What Happens if we Vary K-eff?

For all of the systems discussed above we only considered systems with **fixed K-eff** where the product $\rho * R$ is a constant, and how the time constant (α) and mass vary with density ρ and linear dimensions R. We can take these relationships further by realizing that in the relationship,

$$K-eff = C* \rho * R$$

the constant of proportionality C, is very insensitive to changes in K-eff. In principle this relationship only applies to fixed K-eff, but in practice it says that if we now vary ρ^*R a little, K-eff will also vary a little as a linear function of ρ^*R . Actually as we will see below we can vary ρ^*R quite a bit and still get a linear change in K-eff, e.g., a 10% change in ρ^*R results in about a 10% change in K-eff.

However, the other scaling laws, such as the linear variation of the time constant α with density ρ only applies for fixed ρ^*R and MUST not be used for variable ρ^*R ; this point will be illustrated below where I present results for a system in which for fixed R and an increase in density ρ the time constant α decreases.

These scaling laws can be very powerful when properly applied, but be WARNED that they can lead to completely unrealistic results if used where they do not apply. Therefore it is important that you understand where these laws apply; hopefully by the end of this paper you will understand.

Introduction

We are interested in solving the linear Boltzmann equation, which in its differential form can be written as,

$$\frac{1}{v} \frac{\partial N}{\partial t} + \Omega^* \nabla N + \Sigma t^* N = \iint F(\Omega', E' -> \Omega, E) \ N(\Omega', E') d\Omega' dE' + S$$

$$N(R, \Omega, E, t) = \text{the angular neutron flux}$$

$$v = \text{the neutron speed (speed, not velocity)}$$

$$S(R, \Omega, E, t) = \text{the extraneous (flux independent) source}$$

$$F(R, t, \Omega', E' -> \Omega, E) = \text{the "collision" transfer term}$$

$$\Sigma t(R, E, t) = \text{the total macroscopic neutron interaction cross section}$$

The "collision" transfer term can be written as a sum of reactions, e.g., scatter, fission, (n,2n), (n,3n), etc., any reaction in which one or more neutrons emerges from the reaction,

$$F(R,t,\Omega',E'->\Omega,E) = \sum_k Mk(R,t,E') * \Sigma k(R,t,E') * fk(R,t,\Omega',E'->\Omega,E)$$

$$Mk(R,t,E') = \text{the multiplicity for reaction k, e.g., 1 for elastic, 2 for (n,2n),}$$

$$< v(E') > \text{ for fission}$$

$$\Sigma k(R,t,E') = \text{the macroscopic interaction cross section for reaction k}$$

$$fk(R,t,\Omega',E'->\Omega,E) = \text{the normalized (integrated over } \Omega',E') \text{ probability for reaction k}$$

In this report I will only be interested in criticality problems, in which there is no extraneous source, i.e., S = 0, and this term will be ignored from this point on.

For the definition of integral system parameters, such as K-eff, neutron lifetime τ , and system time constant α , see the appendix. In my earlier report [1] I stated that for ANY spherical, homogeneous, bare system we have the EXACT relationship,

K-eff =
$$C* \rho * R$$

K-eff = K-effective of the system; a constant in this relationship

C = a constant (to be determined)

 ρ = density of the material (grams/cc)

R = radius of the sphere (cm)

What this relationship says is that starting from a given system if we double the density and half the radius to define a new system, the resulting system will have EXACTLY the same K-eff as the original system. We can derive this relationship directly from the Boltzmann equation without any approximations, simply by changing to dimensionless variables, e.g., this is done in many textbooks. In my earlier report I limited conclusions to simple, spherical, bare, homogeneous systems.

This relationship can be generalized to any system, by realizing that if we could change the density and linear dimensions uniformly throughout any system, such that the product remains constant, the same relationship is valid. To see this we can re-write the Boltzmann equation explicitly in general Cartesian coordinates,

$$\frac{1}{v}\frac{\partial N}{\partial t} + \left[\alpha \frac{\partial N}{\partial x} + \beta \frac{\partial N}{\partial y} + \gamma \frac{\partial N}{\partial z}\right] + \rho * A * \sigma t * N = \iint F * N d\Omega' dE'$$

$$F(R,t,\,\Omega',E'->\Omega,E) = \rho * A * \sum_{k} Mk(R,t,E') * \sigma k(R,t,E') * f k(R,t,\Omega',E'->\Omega,E)$$

The microscopic cross sections (Σ) are merely the microscopic (σ) cross sections multiplied by a density (ρ) and a constant (A). In general the cross sections and density will be spatially dependent, such that Σ , σ , ρ , and A are all spatially dependent. Here I will uniformly throughout space divide all terms by some constant factor Θ ,

$$\frac{1}{v}\frac{\partial N}{\Theta\partial t} + \left[\alpha \frac{\partial N}{\Theta\partial x} + \beta \frac{\partial N}{\Theta\partial y} + \gamma \frac{\partial N}{\Theta\partial z}\right] + \frac{\rho}{\Theta} * A * \sigma t * N = \iint F'*Nd\Omega' dE'$$

$$F'(R,t,\Omega',E'->\Omega,E) = \frac{\rho}{\Theta} * A * \sum_{k} Mk(R,t,E') * \sigma k(R,t,E') * f k(R,t,\Omega',E'->\Omega,E)$$

If I define a new density uniformly throughout all space and new dimensions and new time units,

$$\rho'(R,t) = \rho(R,t)/\Theta$$

$$x' = \Theta * x$$

$$y' = \Theta * y$$

$$z' = \Theta * z$$

$$t' = \Theta * t$$

I find an equation that is equivalent to the original equation, as far as neutrons are concerned,

$$\frac{1}{v}\frac{\partial N}{\partial t'} + \left[\alpha \frac{\partial N}{\partial x'} + \beta \frac{\partial N}{\partial y'} + \gamma \frac{\partial N}{\partial z'}\right] + \rho'*A*\sigma t*N = \iint F*Nd\Omega'dE'$$

$$F(R,t,\,\Omega',E'->\Omega,E) = \rho'*A*\sum_{k} Mk(R,t,E')*\sigma k(R,t,E')*fk(R,t,\Omega',E'->\Omega,E)$$

Physically this can be easily understood by noting that neutrons are quite stupid and do not understand grams and cm, but they do understand mean-free-paths. All systems in which the product of density and a linear dimension is a constant will be exactly the same number of mean-free-paths in size, and will have the same properties as far as neutrons are concerned. In other words,

Any property = $C^*[density]^*[linear dimension]$

In particular,

K-eff = $C^* \rho^* R$, where C is the constant of proportionality, to be determined

Time Relationship

For **space** the above results say that as far as neutrons are concerned the same system at different density ρ and linear dimensions R as long as the product $\rho * R$ is constant will be indistinguishable as far as all having the same K-eff, e.g., all time independent variations of a system where we keep $\rho * R$ constant are indistinguishable. However, for **time** they are distinguishable, in the sense that increasing the density shortens the mean-free-path making everything happen faster, which means the time scale is shortened. We have the simple relationship between the system time constant (α) , K-eff, and the neutron lifetime (τ) , [2],

$$\alpha = \frac{K-1}{\tau}$$
, K here is merely a shorthand for K-eff.

If we do change a system such that $\rho * R$ remains constant, even if K-eff is maintained as a constant, increasing the density will shorten the neutron lifetime (τ) , resulting in a larger time constant (α) . So that we also have the relationship,

 $\alpha = D^* \rho$, where D is the constant of proportionality, to be determined

This tells us that any uncertainty or variation in the density (ρ) will have a direct, linear effect on the time constant (α) of the system. Let me stress that this relationship is valid only for fixed $\rho * R$; I will present results below to illustrate this point.

Mass Relationship

The mass of any system is an integral over the density of the system through all space,

$$Mass = \iiint \rho(x, y, z) dx dy dz$$

If I modify the density throughout all space by a factor of $\frac{1}{\Theta}$ and I modify each of the three dimensions of the system by a factor of Θ , I find,

$$Mass2 = \Theta^{2} \iiint \rho(x, y, z) dx dy dz = \Theta^{2} *Mass$$

Since both of these systems will have exactly the same K-eff, we find the general relationship, that for a fixed K-eff, the mass of the system will vary inversely as the square of the density,

$$Mass = A/\Theta^2$$

This relationship tells us is that for any given system if we **perform one transport calculation** at one density and dimensions, to define the constant A, we can easily define the mass at any other density and dimensions where the product of density and linear dimension are a constant.

In my earlier report I presented results for simple, spherical, homogeneous, bare systems, containing plutonium and uranium; for completeness I include results for these systems here. In addition I extend the results to illustrate that this simple scaling law can be used to easily define sensitivity of results to changes in a systems parameters. For example, above I showed that for any given system with a given K-eff, all systems with the same product of $\rho * R$ will have the same K-eff, and the critical mass of these systems will vary as $1/\rho^2$. What I did not mention is that the same system with a different product of $\rho * R$ will have a different K-eff, and a different mass, but the variation of the mass with density will also vary as $1/\rho^2$, producing on a log-log plot a straight line parallel to the line for any other K-eff. The variation from one of these lines to another defines the sensitivity of the systems K-eff to changes in density and dimensions. I will illustrate this point below.

Spherical, Homogeneous, Bare Results

In my earlier report [1] I considered four systems: two PuO2 , one UO2 and one U3O8 system. The compositions of these systems were,

Case	Pu239	Pu240	Pu241	Pu242	O16
#1	0.3116	0.0200	0.0017	0.0000	0.6667
#2	0.2100	0.0756	0.0420	0.0057	0.6667

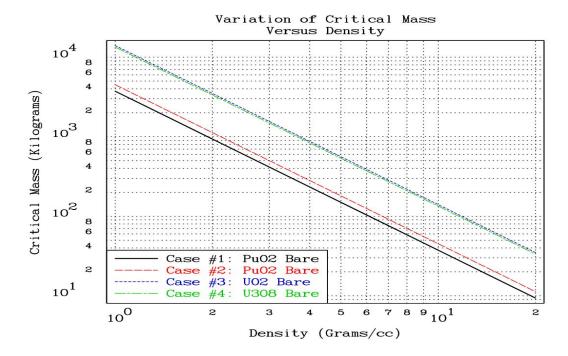
Case	U234	U235	U238	O16
#3	0.0033	0.3100	0.0200	0.6667
#4	0.0027	0.2536	0.0164	0.7273

For my earlier report [1] I run TART [3] static K-eff calculations for a variety of densities to verified the relationships between critical mass and density for these four systems. Here I repeat these calculations including an improved model of the delayed neutron emission spectra [4, 5] to more accurately define the relationships. The results are simple relationships relating the **critical mass in kilograms**, to density ρ in grams/cc and radius R in cm,

Case #1: Mass =
$$3739.5/\rho^2$$
 $\rho*R = 96.2887$ for an exactly critical system Case #2: Mass = $4506.6/\rho^2$ $\rho*R = 102.468$ Case #3: Mass = $14001.8/\rho^2$ $\rho*R = 149.5197$ Case #4: Mass = $13394.8/\rho^2$ $\rho*R = 147.3272$

To illustrate how convenient this simple scaling is, from the above relationships we can see that for system #1, at a density of 10 grams/cc the critical mass is 37.395 kilograms, whereas at a density of 2 grams/cc it is 934.75 kilograms.

Below I illustrate results for these four systems with density between 1 and 20 grams/cc. On this log-log plot we see four straight, parallel lines, making it trivial to determine the critical mass of these systems at any density. For any system(s) that you are interested in you can make similar plots for your use.



Sensitivity

These are the results for exactly critical systems. But we can learn even more by looking at these systems when they are sub or super-critical. For the same composition and geometry we can vary the critical $\rho * R$, reducing it to make the system sub-critical, or increasing it to make the system super-critical.

It is interesting to note that a fractional change in ρ^*R results in a very similar change in K-eff. For example for these systems reducing ρ^*R to 0.9 of its value results in K-eff of about 0.9; similarly increasing ρ^*R to 1.1 of its value results in K-eff of about 1.1.

K-eff based on variations of $\rho * R$

$\% \rho * R$	Case #1	Case #2	Case #3	Case #4
70	0.7051	0.7068	0.7085	0.7044
80	0.8062	0.8073	0.8109	0.8083
90	0.9045	0.9050	0.9083	0.9073
95	0.9526	0.9529	0.9550	0.9546
100	1.0	1.0	1.0	1.0
105	1.0466	1.0462	1.0435	1.0439
110	1.0923	1.0916	1.0857	1.0865
120	1.1809	1.1794	1.1647	1.1661
130	1.2663	1.2631	1.2378	1.2392

The table above illustrates this point for a range of $\rho * R$ from 70% to 130% of its critical value; this table gives more precise values than assuming exact linear dependence

between K-eff and $\rho * R$. The conclusion is that over a fairly wide range of K-eff it is directly proportional to $\rho * R$ with roughly the same constant of proportionality, i.e.,

K-eff =
$$C* \rho * R$$

Here the constant C is fairly insensitive to the value of K-eff. This makes this simple relationship even more useful, because once we determine C by **running only one criticality calculation**, not only can we define variation of a system with the same K-eff based on the same $\rho * R$, but we can also to a good approximation define the K-eff of the same system if we vary $\rho * R$; this means we know the sensitivity of K-eff for the system to changes in $\rho * R$,

$$\frac{\partial K - eff}{\partial [\rho * R]}$$
 = C, with the same constant C, fairly independent of the value of K-eff

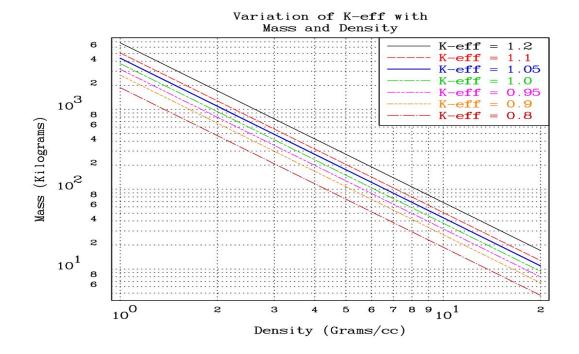
From the table above we do see a definite asymmetry where the sub-critical systems scale more closely as a linear function of $\% \rho * R$ than do the super-critical systems, but still the simple relationship is fairly accurate for a surprisingly wide range of K-eff.

Below I illustrate the variation of K-eff with mass and density corresponding to Case #1 defined above. Here I plot the variation of the Mass for a range of densities between and 1 and 20 grams/cc and a range of K-eff between 0.8 and 1.2. For any given system figures such as this can be quite handy for a number of purposes,

- 1) If you have a system of a fixed mass, a horizontal line on this figure tells you how much you would have to change density for any change in K-eff.
- 2) If you have a system of a fixed density, a vertical line on this figure tells you how much you would have to change the mass for any change in K-eff.

These can be used either to predict what will happen if you do change the system, or they can be used to define safety margins. For example, this system at density 2 grams/cc with a K-eff = 0.9 would have a mass of 671.3 kilograms, whereas a critical system at the same density would have a mass of 934.8 kilograms, indicating a fairly safe margin of 263.5 kilograms; almost 40% of the current mass. As a second example, if this system at 2 grams/cc with a K-eff = 0.9 were compressed to 2.40 grams/cc it would become critical; a 20% increase in the current density.

Because of our simple scaling law results such as this can be obtained for any system based on **just a few transport calculations**, **at fixed densities**, and the results can then be generalized to produce figures such as the one shown here.



I will again mention the importance of understanding where these scaling laws apply and using them properly. Below I give examples of where these scaling laws do and do not apply.

Scaling with Constant $\rho * R$

The following results are for Case #1 in a critical state. Here I show large (order of magnitude) changes in ρ and R, in order to illustrate that scaling is exact over any range as long as the product $\rho * R$ is constant. Rates are in units of events per μ sec. and counts (#) are normalized per neutron removed.

R ρ	96.2887 1.0	9.62887 10.	0.962887 100.
Mass (kg)	3739.5	37.395	0.37395
Rem. Rate	12.6502	126.502	1265.02
Abs. Rate	4.2738	42.738	427.38
Leak. Rate	8.3764	83.764	837.64
Prod. Rate	12.6489	126.489	1264.89
Rem. #	1.0	1.0	1.0
Abs. #	0.3379	0.3379	0.3379
Leak. #	0.6621	0.6621	0.6621
Prod. # (K)	1.0000	1.0000	1.0000

In this case: K-eff is the independent of ρ , since the counts (#) are independent of ρ , Mass scales as $1/\rho^2$, and rates scale linearly with ρ . The linear scaling of the rates means that the time constant (α) of the system is scaling linearly with ρ . This is yet another confirmation of the scaling laws for constant $\rho * R$.

Scaling with Variable $\rho * R$

The following results are for Case #1 in a sub-critical, critical, and super-critical state. Here I maintained R as constant and made relatively small 10 % changes in ρ , i.e., 90%, 100% and 110% of the critical $\rho * R$. Rates are in units of events per μ sec. and counts (#) are normalized per neutron removed.

R ρ	9.62887 9.	9.62887 10.	9.62887 11.
Mass (kg)	33.655	37.395	41.134
Rem. Rate	129.001	126.502	124.441
Abs. Rate	39.313	42.738	46.043
Leak. Rate	89.688	83.764	78.398
Prod. Rate	116.661	126.489	135.929
Rem. #	1.0	1.0	1.0
Abs. #	0.3047	0.3379	0.3700
Leak. #	0.6952	0.6621	0.6299
Prod. # (K)	0.9043	1.0000	1.0923

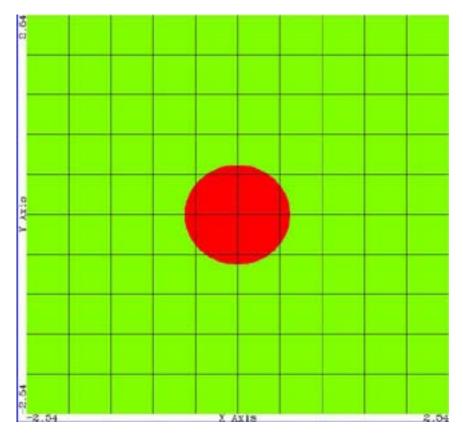
The linear scaling of K-eff with $\rho * R$ is still fairly accurate. But we see a contradict for other scaling laws, for example, our scaling laws predict that all of the rates should increase as a linearly function of ρ , and instead here we see some are actually decreasing. This is because as we increase ρ the absorption and production rates are increasing due to the reduction in mean-free-path, but the leakage is decreasing because the system is more mean-free-paths thick. This is a leakage dominated system (roughly 2/3 of the neutrons produced leak), so the effect is obvious. In general for fixed R there is no simple relationship between changes of density ρ and the system time constant α .

Hopefully this will serve as a **WARNING to only use the scaling laws where they accurately apply**. As a summary,

- 1) The scaling laws always work for constant $\rho * R$.
- 2) K-eff scales fairly accurately with variable $\rho * R$.
- 3) Time constant α scales ONLY for constant $\rho * R$.

General Scaling

The above examples are the same as the geometrically simple examples presented in my earlier report [1], here extended to include the description of sensitivity. Next I consider the generalization to more complicated geometry. In a recent study we examined a set of theoretical pin cells [6]. The set of pin cells consisted of cylindrical uranium pins 1/2", 1/4" and 1/8" in radius surrounded by water. Each cell has 2" pitch, and the cells infinitely repeat in all directions, so there is no leakage. The below figure illustrates one of these pin cells, with the uranium pin (red) centered in the water (green).



To illustrate the general scaling law I randomly selected the 1/2" radius pin cell problem, which is defined as follows; the **bold** quantities are those of interest for this comparison, i.e., dimensions and densities.

Problem #1 1/2" (1.27 cm) radius fuel pin – 18.8 grams/cc density – total $\langle v \rangle$ - static criticality 99.02 atoms of U²³⁸ to 0.98 atoms of U²³⁵ 2" square water – 1.0 grams/cc density

I then halved the density and doubled the dimensions to define a second pin cell,

2.0 atoms of hydrogen to 1.0 atoms of oxygen

```
Problem #2

1" (2.54 cm) radius fuel pin –

9.4 grams/cc density – total < v > - static criticality
99.02 atoms of U 238 to 0.98 atoms of U 235

4" square water -

0.5 grams/cc density
2.0 atoms of hydrogen to 1.0 atoms of oxygen
```

TART calculations confirmed that both of these systems have the same K-eff, they differ in that compared to Problem, #1, the time constant (α) for the Problem #2 is half that of Problem #1, and the mass per cell is four times as large, as predicted above based on density scaling. I repeated calculations with up to factors of ten changes in density and dimensions such that the product remained constant, and again verified that the scaled systems have the same K-eff as the original system and the that the time constant (α) correctly scales. These results illustrate that the scaling laws apply to any geometry, not just simple bare, homogeneous spheres covered in my earlier report [1].

Reflected Systems

This topic was covered in my earlier paper [1] and will not be repeated in detail here; I will mention only a few important points. If we are interested in uniformly changing density and dimensions throughout a system we can use the simple $\rho * R$ scaling laws defined above. However, if we are only interested in changing density of the fuel portion of a system that is surrounded by a reflector, unfortunately there is no simple EXACT solution for this problem.

The subject of reflected systems has been studied and results published for the over half a century; see for example, Enrico Fermi's work published in 1945 [7]. In this report Fermi refers to even earlier work by Robert Oppenheimer. Even at that time the scaling laws for simple systems were well understand, and had been extended to reflected systems. Reflected system will obey the $1/\rho^2$ variation described here, as long as the entire system is scaled. However, if only the inner portion of the system is scaled, but not the reflector, it has been empirically determined that well reflected systems scale close to $1/\rho^{1.5}$. For example, we can compare the four systems described above bare and surrounded by 10 cm of water.

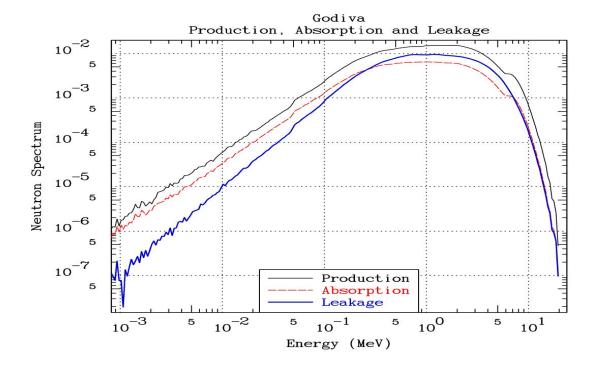
Bare (same results as above)	
Case #1: Mass = $3739.5/\rho^2$	$467/\rho^{1.5}$
Case #2: Mass = $4506.6/\rho^2$	$619/\rho^{1.5}$
Case #3: Mass = $14001.8/\rho^2$	$1661/\rho^{1.5}$
Case #4: Mass = $13394.8/\rho^2$	$1770/\rho^{1.5}$

Here we see a large reduction in critical mass when a reflector is added to these systems. Note, that for the bare systems the critical mass of Case #4 is slightly less than that of Case #3, whereas for the reflected systems the critical mass of Case #4 is slightly more than that of Case #3.

A Simple, Real System: Godiva

As a simple example of how these scaling laws can be used, consider Godiva, which is a highly enriched uranium, fast neutron, critical system. There are actually many models of this system, so I will not give the exact details of which model I used. For this example it is sufficient to consider Godiva at two different temperatures: 300 Kelvin and 600 Kelvin. This system is very fast, with essentially no low energy neutrons; see the below plot that illustrates nothing is happening below 1 keV or even 10 keV. Therefore the change in temperature will have a negligible effect on the neutron cross sections of interest.

In this case the dominant effect of temperature will be to change the density of the uranium. For this example I use for the uranium density 18.8344~grams/cc at 300~Kelvin, and 18.55076~grams/cc at 600~Kelvin [8]. For this system I calculate that the critical $\rho*R$ is 163.23265, so that the critical radius is 8.66673~cm 300 Kelvin and 8.79924~cm at 600~Kelvin. The results are critical masses of 51.358~kg at 300~Kelvin and 52.940~kg at 600~Kelvin, a difference of 1582~grams, or 5.27~grams/degree Kelvin. There are a few conclusions we can draw: 1) Based on thermal expansion this system is safe, in the sense of having a negative Doppler coefficient, i.e., if the system is critical at 300~Kelvin, as it heats up it will expand and become sub-critical, 2) For this system the quoted uncertainty is 20~grams. There are many factors that contribute to the uncertainty of the critical mass, but we can see that a mere 4 degree Kelvin change in temperature would correspond to over 20~grams; this makes the quoted uncertainty appear to be overly optimistic.



Uncertainties

In using results of any transport calculation it is important to understand the uncertainties in the model used and in the results. Contributing factors to uncertainties are discussed in detail in my earlier report [1] and for completeness will be repeated here. The per-cent uncertainties here refer to the critical mass.

- 1) The TART transport calculations were run to a high degree of accuracy, and should not introduce any additional uncertainty.
- 2) I estimate that the nuclear data introduces an uncertainty of about 3 to 5%.
- 3) The results will be a function of temperature. Here all calculations were based on room temperature. Anyone who has ever held a ball of plutonium in their hand knows that due to alpha decay, it is not at room temperature. Fortunately, reasonably small variations from room temperature (as with plutonium) will have a very small effect on the results.
- 4) Here I modeled each system as completely isolated, surrounded only by vacuum, which means no reflection. "Room return" can have a major effect on results; I estimate up to 10%.
- 5) Here I modeled the reflector as pure water. The critical mass will be very sensitive to any impurities in the reflector that can absorb neutrons. The uncertainty introduced by this assumption is hard to quantify, because of the wide variety of available reflector materials and their impurities, but it is fair to say that it will be at the few per-cent level.
- 6) Isotopics can be a major source of uncertainty. If you are interested in ONLY EXACTLY the composition considered here, there is no uncertainty. However, if you are really interested in a the critical mass of a range of real systems that you might encounter, you should be aware that the critical mass is very strongly dependent on: a) additional scatterers, as can be seen above for UO2 versus U3O8, and b) how much neutron poison is included in the composition: for Pu, Pu240, Pu242, and for U, U234, U236, U238. To illustrate this last effect I considered the limiting cases of pure Pu239 for the Pu systems or U235 for the U systems.

Case #1: Mass =
$$3739.5/\rho^2$$
 pure Pu239 = $3573/\rho^2$
Case #2: Mass = $4506.6/\rho^2$ "
Case #3: Mass = $14001.8/\rho^2$ pure U235 = $12308/\rho^2$ "
Case #4: Mass = $13394.8/\rho^2$ "

Conclusion

By understanding the simple scaling relationships a great deal of insight can be gained regarding any system, and how its reactivity will change based on changes in its linear dimensions, density or mass. Once you understand these scaling laws you will realize that this insight can be gained after running a rather small number of transport calculations;

since we now know that results based on any given density can be generalized to any other density.

But again, be WARNED to use these scaling laws only where they apply. Failure to heed this WARNING can lead to completely unrealistic results, e.g., it is incorrect to assume that the time constant α always increases with density ρ ; above I presented a case where just the opposite is true.

Acknowledgements

I thank Chris Clouse, LLNL, for reviewing a draft of this paper, and in particular for pointing out the importance of understanding where these scaling laws accurately apply, and insuring that they are properly used. Chris' contributions have considerable improved this paper, and hopefully made it easier for readers to understand. I also thank Dave Heinrichs for pointing out the reference to Enrico Fermi's work [7] and for supplying the temperature dependent uranium density used in the Godiva example.

Appendix: Definition of Integral Parameters, K-eff, lifetime τ and time constant α

For time independent codes there is a very simple textbook definition that can be used to define K-eff. It is the ratio of the number of neutrons produced by fission in one generation to the number produced in the preceding generation; these codes need not consider anything else. For time dependent codes or codes that define K-eff in terms of a balance between neutrons produced and removed the definition is more complicated, but it allows us to see the true basic definition.

Starting from the time dependent, linear Boltzmann equation in general geometry,

$$\frac{1}{v}\frac{\partial N}{\partial t} + \Omega * \nabla N + \Sigma t * N = \iint (\langle v \rangle \Sigma f + \Sigma scatter + 2\Sigma n, 2n + 3\Sigma n, 3n +) Nd\Omega' dE'$$

Where $N(r,\Omega,E,t)$ is the neutron flux, $v*n(r,\Omega,E,t)$, v is the neutron speed, Σt is the macroscopic total cross section, $\langle v \rangle$ is the average number of neutrons emitted per fission, Σf , $\Sigma scatter$, $\Sigma n,2n$, $\Sigma n,3n$, etc., are the macroscopic cross sections for each type of event. For simplicity I will use neutron density $n(r,\Omega,E,t)$ in the following,

Integrate over all space, energy, and direction

$$\frac{\partial n}{\partial t} + \left[L^*v^*n\right] + \left[\Sigma t^*v^*n\right] = \left[(< v > \Sigma f + \Sigma scatter + 2\Sigma n, 2n + 3\Sigma n, 3n + \dots)v^*n\right]$$

Collecting terms together we find a simple equation defining the time dependent behavior of the system,

$$\frac{\partial n}{\partial t} = \alpha * n$$

$$\alpha = \left[(\langle v \rangle \Sigma f + \Sigma scatter + 2\Sigma n, 2n + 3\Sigma n, 3n +)v \right] - \left[L^*v \right] - \left[\Sigma t^*v \right]$$

Scatter does not directly effect the balance of neutrons or the definition of α and can be subtract. Upon defining the absorption cross section: $\Sigma a = \Sigma t - \Sigma scatter$, we find,

$$\alpha = [(\langle v \rangle \Sigma f + 2\Sigma n, 2n + 3\Sigma n, 3n +)v] - [L*v] - [\Sigma a*v]$$

- = [Production rate] [Leakage Rate] [Absorption Rate]
- = [Production rate] [Removal rate]; Removal = Leakage + Absorption

This is the most general definition of α defined in terms of the neutron balance of the system, based upon neutron production, leakage, and absorption **rates**. However, we will take this definition further,

$$\alpha = \left[\frac{\text{Pr} oductionRate}{\text{Re} movalRate} - 1\right] * [\text{Removal Rate}]$$

We define

$$K\text{-eff} = \frac{\Pr{oductionRate}}{Re\,movalRate} = \frac{\Pr{oduction\#}}{Re\,moval\#}$$

$$\tau = 1/[Removal Rate] = Neutron lifetime$$

to find the form normally used,

$$\alpha = \frac{K-1}{\tau}$$

Note, that the ratio of production and removal rates eliminates time, and allows us to express K-eff either in terms of rates or simply in terms of events (#) without reference to time, which is how time independent codes define it.

Hopefully the above derivation allow you to see where the forms normally used come from and at the same time allows you to see the most general definition of the system time constant α in terms of production, leakage and absorption rates; in particular note that in this form α can be defined directly without the use of K-eff or neutron lifetime.

References

- [1] "Mass and Density, Criticality Relationships", Lawrence Livermore National Laboratory, UCRL-ID-143496, April, 2001, by D.E. Cullen
- [2] "Static and Dynamic Criticality: Are they different?", Lawrence Livermore National Laboratory, UCRL-TR-201506, November 2003 by D.E. Cullen, et. al. now available online at http://www.llnl.gov/cullen1/crits1.htm
- [3] "TART 2002: A Coupled Neutron-Photon 3-D, Combinatorial Geometry Time Dependent Monte Carlo Transport Code," Lawrence Livermore National Laboratory, UCRL-ID-126455, Rev. 4, November, 2002, by D.E. Cullen; documentation available on-line at http://www.llnl.gov/cullen1/mc.htm. This is the most recent public release of TART, but it does not include the delayed neutron model described here; see [4] below.
- [4] "A Simple Model of Delayed Neutron Emission," Lawrence Livermore National Laboratory, June 2004, UCRL-TR-204743, by D.E. Cullen; documentation available online at http://www.llnl.gov/cullen1/delayed.htm
- [5] "TART 2004: A Coupled Neutron-Photon 3-D, Combinatorial Geometry Time Dependent Monte Carlo Transport Code," to be published, by D.E. Cullen. The delayed neutron model used here is available in TART04-3 and all later versions of TART; regarding availability contact D.E.Cullen <u>cullen1@llnl.gov</u>.
- [6] "How Accurately can Calculate Thermal Systems", Lawrence Livermore National Laboratory, UCRL-ID-126455, Rev. 4, April, 2004, by D.E. Cullen and many others; documentation available on-line at http://www.llnl.gov/cullen1/pin_cell.htm
- [7] "Critical Mass Measurements for a 25 Sphere in Tu and WC Tampers", by E. Fermi, et. al., LA-442, October 1945. I am indebted to Dave Heinrichs for pointing out this reference to me.
- [8] The temperature dependent uranium densities are based on a Private Communications, Dave Heinrichs, Lawrence Livermore National Laboratory, 2004.

University of California	
Lawrence Livermore National Laboratory	
Technical Information Department	
Livermore, CA 94551	
	_